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Comparison of Moliere scattering theory with Mott scattering in liquid hydrogen

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We examine multiple scattering in liquid hydrogen by direct simulation of multiple single scattering events. We use the Mott cross section modified by atomic and nuclear form factors to model single scattering events. The computed total elastic cross section and the resulting value for the mean free path between elastic collisions agrees well with other similar calculations. The spatial angle distribution agrees approximately with Moliere theory when the number of collisions in the material corresponds to the parameter Ω_o expected in the theory. However, detailed examination of the shape of the angular distribution using the total cross section determined here suggests that the Moliere theory may underestimate the scattering probability in hydrogen.

1 Introduction

Accurate modeling of ionization cooling in the muon collider depends critically on a precise description of multiple scattering. In a previous paper [1] we showed that Moliere theory is suspect for materials with $Z<4$. Comparison of the theory with the few experimental results available suggested a discrepancy with theory for Be and Li. No experimental results on the angular spectrum were available for hydrogen, which is the best material for ionization cooling. On the other hand hydrogen is the simplest and best understood material theoretically. Thus we are lead to consider checking the Moliere theory by directly comparing predictions of the spatial scattering angle with the angle resulting from a large number of simulated Mott scatterings. Similar calculations have also been done by Paul Lebrun [2].

2 Mott scattering

The electromagnetic scattering of a charged particle from the nucleus of some material is given by the Rutherford cross section

$$\frac{d\sigma}{d\Omega_R} = \frac{Z^2}{4} r_e^2 \left(\frac{m_e c^2}{p\beta c} \right)^2 \frac{1}{\sin^4 \frac{\theta}{2}} \qquad \textbf{(1)}$$

In this equation Z is the atomic number, β is the velocity over c, p is the muon momentum, m is the mass of the muon and r_e is the classical radius of the electron. This equation is appropriate either in the Center of Momentum (CM) frame of the beam and target particles or else approximately in the Laboratory (LAB) frame when the target is much heavier than the incident particle. Mott determined a relativistic correction to the Rutherford cross section for spin ½ incident particles, given by

$$\frac{d\sigma}{d\Omega_M} = \frac{d\sigma}{d\Omega_R} \left(1 - \beta^2 \sin^2 \frac{\theta}{2} \right) \qquad \textbf{(2)}$$

The spin of the target nucleus is ignored. In order to account for the screening of the nuclear charge by the atomic electrons, the Mott cross section must be multiplied by an atomic elastic form factor [3]

$$F(q) = \frac{1}{\left[1 + \left(\frac{a_o q}{2\hbar c} \right)^2 \right]^2} \qquad \textbf{(3)}$$

where a_o is the Bohr radius. The momentum transfer q is related to the elastic scattering angle by

$$q(\theta) = \sqrt{2}\, p \, \{1 - \cos\theta\}^{1/2} \qquad \textbf{(4)}$$

Thus this factor primarily affects the small angle behavior of the cross section. The large angle behavior is affected by the nuclear form factor [4]

$$F_N = \frac{1}{\left[1 + \left(\frac{\theta}{\theta_N} \right)^2 \right]^4} \qquad \textbf{(5)}$$

where the characteristic angle is

$$\theta_N = \frac{\lambda'}{R_N} = \frac{140.7}{p[MeV/c]\ A^{\frac{1}{3}}} \quad \textbf{(6)}$$

In this relation λ' is the deBroglie wavelength divided by 2π.

3 Transformation to LAB frame

Even though the ratio of the muon to hydrogen atom masses is only ~11%, target recoil effects can have a noticeable effect on the scattering angle distributions. The LAB angle ψ corresponding to a given CM angle θ is given by [5]

$$\tan\psi = \frac{\sin\theta}{\gamma_{CM}(\cos\theta + g^*)} \quad \textbf{(7)}$$

The parameter g* is given by

$$g^* = \frac{\beta_{CM}}{\beta_1^*} \quad \textbf{(8)}$$

where β_{CM} is the velocity of the CM frame in the LAB and β_1^* is the velocity of the muon in the CM frame. The two angles are the same for 0° and 180°, but diverge by up to ~11° for angles near 90°. When the parameter g* is greater than 1, the maximum angle in the LAB frame is limited to

$$\psi_{max} = \tan^{-1}\frac{1}{\gamma_{CM}\sqrt{g^{*2}-1}} \quad \textbf{(9)}$$

The maximum LAB angle is 180° for a single μH scattering, but only 0.28° for a single μe scattering.

4 Total elastic cross section

In order to model multiple scattering as a series of single scattering events, we need to know the mean free path for elastic scattering in the material. This is given by

$$\lambda_{int} = \frac{1}{n_a \sigma_{tot}} \tag{10}$$

where σ_{tot} is the total elastic cross section and

$$n_a = \frac{N_A \rho}{A} \tag{11}$$

is the number of atoms per unit volume. N_A is Avogadro's number and {ρ, A} are the {density, atomic weight} of hydrogen. $n_a = 4.23\ 10^{22}$ / cm^3 in liquid hydrogen in the LAB frame.

A theoretical estimate of the total elastic cross section, given by Mott and Massey [7], is

$$\sigma_{tot} = \frac{1024\ \pi^5 m^2 e^4}{3 h^4} \frac{(3\lambda^4 + 18\ \lambda^2 k^2 + 28\ k^4)}{\lambda^2 (\lambda^2 + 4 k^2)^3} \tag{12}$$

where

$$k = \frac{m v}{\hbar}$$
$$\lambda = \frac{2}{a_o} \tag{13}$$

Another theoretical estimate, given by Jackson [8], is

$$\sigma_{tot} = \pi a_o^2 \left(\frac{2 Z e^2}{\hbar v} \right)^2 \tag{14}$$

It is also possible to compute the total cross section by numerically integrating the differential cross section over all angles. This is a delicate numerical problem since the function being integrated differs in value by more than 20 orders of magnitude over its range.

Since the total cross section is a Lorentz invariant quantity, we can evaluate it in the CM frame.

$$\sigma_{tot} = \int_0^{\pi} \frac{d\sigma^*}{d\Omega^*} \, d\Omega^* \qquad \textbf{(15)}$$

We use asterisk superscripts to denote CM quantities. We have successfully integrated the screened Mott cross section and find the total cross section is 1.61 x 10^{-20} cm^2 for a muon momentum of 186 MeV/c. The total cross section is insensitive to upper limits on the integral above 10^{-3} radians. Changing the lower limit from 10^{-8} to 10^{-6} radians changes the integral by 2 parts in 1000. This value of the total cross section gives an interaction mean free path of 1.47 x 10^{-3} cm in the LAB frame. A similar, but independent, calculation has been done by Lebrun [2]. Table 1 shows the results of these calculations expressed in terms of the mean number of collisions in 64 cm of liquid hydrogen. Also shown is the corresponding parameter Ω_o from Moliere theory for scattering from the nucleus (i.e. ignoring any contribution from electron scattering).

Table 1 Mean number of collisions in 64 cm of hydrogen	
Mott & Massey	9.6 K
Jackson	67.4 K
Lebrun	47.6 K
This work	43.7 K
Moliere theory (Z^2)	40.0 K

The mean number of collisions differ by a factor of about 4 among these five calculations. However, the two direct simulations and the Moliere calculation agree to ±10 %.

5 Scattering simulations

We have carried out a simulation of the spatial angular distribution resulting from scattering in 64 cm of liquid hydrogen in a field free region. We computed the cumulative distribution function $F(\theta)$ by integrating the screened differential cross section in double precision from 0 up to the angle θ.

$$F(\theta) = \frac{1}{\sigma_{tot}} \int_0^{\theta} \frac{d\sigma^*}{d\Omega^*} \, d\Omega^* \qquad \textbf{(16)}$$

We used the inverse transformation method [9] to randomly select CM angles from the Mott distribution. Each double precision random number was used in a polynomial interpolation of the distribution function. The simulations used 100K individual muon “tracks”. Each track was forced

to undergo a large number of "interactions" corresponding to the mean number of expected collisions. At each interaction the spatial (polar) angle change θ_i was sampled from the Mott distribution. The CM polar angle was converted to the corresponding LAB angle using Eq. 7. The azimuthal angle φ_i for the same interaction was sampled from a uniform distribution. These quantities were used to calculate the changes in the projected angles using the relations

$$\begin{aligned} \psi_{XZ} &= \tan^{-1}(\tan\psi_i \cos\varphi_i) \\ \psi_{YZ} &= \tan^{-1}(\tan\psi_i \sin\varphi_i) \end{aligned} \qquad \textbf{(17)}$$

The changes in projected angles could be simply added for all interactions to get the cumulative projected angles for the total thickness of the material. After all the interactions the resultant spatial angle could then be computed from

$$\psi = \tan^{-1}\sqrt{\tan^2\psi_{XZ} + \tan^2\psi_{YZ}} \qquad \textbf{(18)}$$

The full trigonometric form of these relations were kept throughout (i.e. no small angle approximations were made) in order not to bias the results at large angles.

Fig. 1 shows a comparison of the Mott scattering simulation with the results of Moliere theory for the case where the nuclear form factor, but not the target recoil, is included in the direct simulation.. The number of collisions used corresponds to that expected in Moliere theory with the Z(Z+1) factor for nuclear and electron scattering. As expected, there is a noticeable decrease due to the nuclear form factor beginning at an angle around 150 mr in the number of large angle scatters compared to Moliere theory. The overall agreement is fairly good. This shows that the Moliere theory accurately models scattering in liquid hydrogen provided (1) Ω_o is an accurate measure of the number of collisions in the material, (2) the multiple scattering distribution from the atomic electrons and the nucleus are the same, and (3) target recoil and nuclear form factor effects are not important.

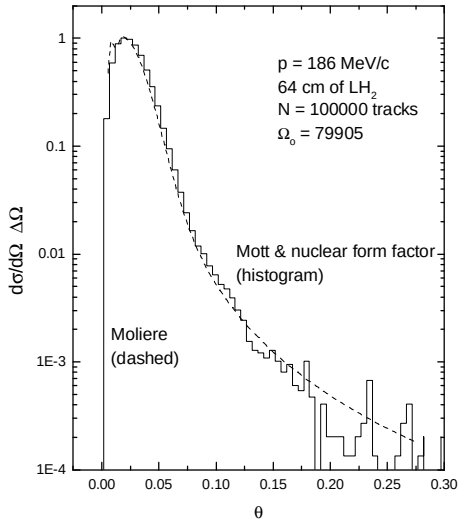

Fig. 1 Comparison of Moliere theory with direct simulation of screened Mott scattering. Nuclear form factor is included, but target recoil effects are not. Data is renormalized to a peak value of 1.

Previous comparisons [10] of Moliere theory with direct simulations of screened Rutherford scattering of 1 MeV electrons also showed good agreement for scattering in carbon, aluminum, and gold. A comparison by Lebrun [2] of 190 MeV/c muons in beryllium showed a complicated dependence where Moliere theory in GEANT3 underestimated scattering angles from 2-3 times the *rms* value, but overestimated the large angle tail. His simulations for hydrogen showed that the screened Mott scattering was narrower than the Moliere prediction.

The properties of the tails of the distributions for these two cases are compared in Table 2.

Table 2 Tail properties		
	N > 0.300	θ_{MAX}
no nuclear form factor	57	0.57
with nuclear form factor	10	0.35

The second column gives the number of events out of 100K that have scattering angles larger than 0.3 radians. The last column gives the largest resultant angle for any track in the simulation.

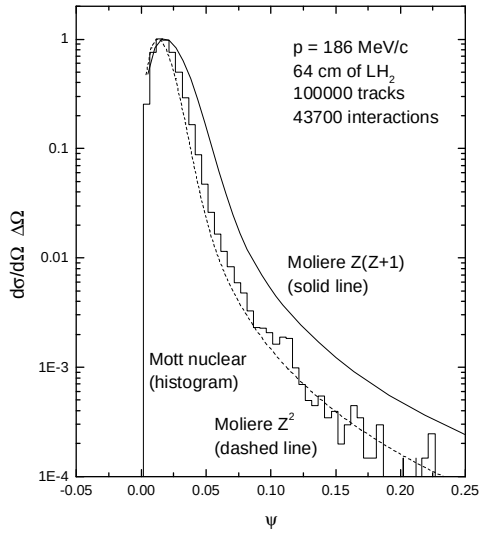

Fig. 2 Comparison of Moliere theory and direct simulation of Mott scattering from the nucleus. Nuclear form factor and target recoil effects are included. Data is renormalized to a peak value of 1.

Fig. 2 shows a comparison of Moliere theory with the direct Mott simulation results, including both nuclear form factor and target recoil effects. Here the number of collisions is determined from the total cross section calculation in Table 1. In other words we are only considering the scattering from the nucleus here and are ignoring the electron contribution. We see that the Moliere calculation underestimates the scattering in the region up to ~2.5 times the *rms* value by ~50%.

One way the Moliere spectrum could be modified is to introduce a correction factor f in the definition of the Moliere characteristic angle parameter

$$\begin{aligned} \chi_C^2 &= 4\pi\, f\, N_A r_e^2 (m_e c^2)^2 \frac{\rho t}{A} \frac{Z^2}{(p\beta c)^2} \\ &= 0.157\, f\, \frac{\rho t}{A} \frac{Z^2}{(p\beta c)^2} \end{aligned} \qquad \textbf{(19)}$$

A value $f = 1.17$ is required to bring the Moliere theory into agreement with the nuclear Mott scattering simulation data in Fig. 2.

6 Discussion

We have computed the total elastic cross section in hydrogen and shown that it agrees with Moliere theory and with an independent calculation by Lebrun. We have shown that Moliere theory agrees with direct simulations of the scattering angle distribution in liquid hydrogen, assuming (1) the theory gives the correct result for the mean number of collisions, (2) multiple scattering from the nucleus and the electron cloud have identical angular distributions in the LAB, and (3) that nuclear form factor and target recoil effects are not important.

The Moliere calculation (as modified by Bethe) assumes that the angular distribution from multiple scattering off the electron cloud is the same as that from the nucleus. This is a very poor approximation in the LAB frame when the expected number of collisions is small (e.g. ~20, which is the quoted lower limit for the validity of Moliere theory). The electron scattering contribution is introduced by changing a multiplicative factor from Z^2 to Z(Z+1), which is a factor of 2 in hydrogen. This factor enters directly into the parameter Ω_o, which corresponds to the mean number of collisions. Lynch and Dahl [11] have discussed this question and point out that the high precision measurements of Shen et al [12] of the *rms* width for hydrogen agreed with Moliere theory with the Z(Z+1) factor present. On the other hand Tollestrup [13] has emphasized the radically different kinematics for μe versus μp scattering at 186 MeV/c.

Comparisons of the shapes of the angular spectra for scattering in the region up to 3 times the *rms* value suggests that Moliere theory underestimates the scattering probability. This appears to be the case for the simulations in hydrogen (cf. Fig. 2, this paper). It also appears to be true for the measured scattering from both the nucleus and the electrons in lithium [1] and beryllium [1,2].

Notes and references

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